MEASUREMENT OF CHARGE EXCHANGE AND X-RAY EMISSION CROSS SECTIONS FOR SOLAR WIND-COMET INTERACTIONS

J. B. Greenwood, I. D. Williams, S. J. Smith, And A. Chutjian Received 2000 January 31; accepted 2000 March 3; published 2000 April 05

ABSTRACT

X-ray emission from a comet was observed for the first time in 1996. One of the mechanisms believed to be contributing to this surprisingly strong emission is the interaction of highly charged solar wind ions with cometary gases. Reported herein are total absolute charge-exchange and normalized line-emission (X-ray) cross sections for collisions of high-charge state (+3 to +10) C, N, O, and Ne ions with the cometary species H_2O and CO_2 . It is found that in several cases the double charge-exchange cross sections can be large, and in the case of C^{3+} they are equal to those for single charge exchange. Present results are compared to cross section values used in recent comet models. The importance of applying accurate cross sections, including double charge exchange, to obtain absolute line-emission intensities is emphasized.

Subject headings: atomic processes — comets: general — X-rays: general

1. INTRODUCTION

A surprising observation was made in 1996 of X-ray emissions from comet Hyukatake using the ROSAT satellite (Lisse et al. 1996). The emission peaked along the Sun-comet line and had a total luminosity of 4×10^{15} ergs s⁻¹, which varied by up to a factor of 4 over a timescale of several hours. Subsequent analysis of the ROSAT All-Sky Survey (1990–1991) by Dennerl, Englhauser, & Trumper (1997) revealed emission from several other comets, suggesting that this is a common phenomenon. A number of theories such as collisions of the comet with interplanetary dust, solar X-ray scattering and fluorescence, and bremsstrahlung from energetic electrons in the coma have been put forward to explain this emission. However, only two models are capable of reproducing the X-ray intensities seen in these observations. These are: (1) charge exchange of heavy solar wind ions with cometary species (Cravens 1997) and (2) scattering of solar X-rays from attogram dust particles (Krasnopolsky 1997). The strongest evidence for the dust scattering model has been given by Owens et al. (1999) from observations of Hale-Bopp by the BeppoSAX and Extreme Ultraviolet Explorer satellites.

The proposed charge-exchange mechanism proceeds as follows (Cravens 1997):

$$A^{q+} + X \to [A^{(q-i)+}]^* + X^{i+} \to A^{(q-j)+} + X^{k+} + (k-j)e^- + N h\nu,$$
 (1)

where *i* electrons are captured by a solar wind ion A^{q+} from the cometary atom or molecule X, leaving the ion in an excited state. Its subsequent decay yields *N* photons. If the initial ion is highly charged, some of these photons will be in the X-ray region. Using the relative abundance of solar wind ions (Bame 1972; Boschler 1987), Cravens selected ions that would generate photons in the energy range observed by *ROSAT*. Assuming that each of these ions produces on average one 200 eV photon, he developed a simple model for the X-ray emission from Hyukatake. For all species considered, a cross section of 3×10^{-15} cm² was used, based on measurements in H and H₂

by Phaneuf et al. (1982) and Dijkkamp et al. (1985). It was also assumed that the fraction of collisions producing an X-ray transition was 10% (an effectivity of f = 0.1). The calculated luminosity of 2×10^{15} ergs s⁻¹ was within a factor of 2 of the *ROSAT* observations.

Häberli et al. (1997) extended this idea to look at individual spectral lines produced from C, O, and Ne ions. The excited state of the ion following capture was assumed to have a principal quantum number $n=q^{0.75}$ followed by a cascading decay of $\Delta n=1$. Cross sections for the C and O ions were from measurements of Phaneuf et al. (1982) for collisions in H and H₂, while a value of 4×10^{-15} cm² for Ne ions was assumed.

By considering individual ions, a synthetic spectrum was produced. The X-ray luminosity from this calculation was 2.7×10^{16} ergs s⁻¹, about 10 times the Cravens value. By considering a wider range of solar wind ions (charge states of C, N, O, Ne, Si, and Fe, using solar wind data of Bame and Boschler), Wegmann et al. (1998) also produced a synthetic spectrum. They used a classical overbarrier model (Mann, Folkmann, & Beyer 1981) to determine total cross sections and the initial excited state of the charge-exchanged ion. In this case, line intensity ratios were assumed to be equal for each ion and an effectivity of f = 0.4–0.8 was applied. This model yielded a luminosity of 1.2×10^{16} ergs s⁻¹. It demonstrated that when enough ions are considered, the spectrum will resemble continuous bremsstrahlung emission as observed by low-resolution detectors, such as those aboard *ROSAT*.

It is clear that models of charge-exchange interaction of the solar wind with the comet can account for the intensity of the X-rays. However, in an effort to determine if it is the *dominant* process, a number of factors make accurate calculations difficult. These are: (1) the value of the cross sections for individual ions in cometary atoms and molecules (such as H₂O, CO₂, CO, OH, and O) are presently unknown; (2) the relative intensities (obtained from line-emission cross sections) and effectivity *f* of the X-ray emission following capture of an electron have not been given detailed consideration; and (3) the density, composition, and variability of the minor solar wind ions are not known in detail.

With the recent launch of the *Chandra* and *X-ray Multi-Mirror* (*XMM*) satellites, unprecedented angular and spectral resolution of cometary X-ray emission will become available. These data should determine the relative importance of the

¹ Physics Department, Queen's University of Belfast, Belfast, BT7 INN, UK; j.greenwood@qub.ac.uk, i.williams@qub.ac.uk.

² Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109; steven.j.smith@jpl.nasa.gov, ara.chutjian@jpl.nasa.gov.

 $TABLE\ 1$ Total Cross Sections for Single and Double Charge Exchange of Various Solar Wind Ions in H,O and CO,

Ion	¹³ C ³⁺	$^{13}C^{6+}$	$^{15}N^{7+}$	¹⁶ O ⁵⁺	¹⁸ O ⁷⁺	$^{18}O^{8+}$	²² Ne ⁹⁺	
H ₂ O:								
$\sigma_{q, q-1}$	1.5 ± 0.1	6.0 ± 1.4	9.5 ± 1.4	4.3 ± 0.5	5.3 ± 0.8	6.3 ± 0.7	8.0 ± 2.0	
$\sigma_{q,\;q-2}^{q,\;q}$	0.8 ± 0.1	0.8 ± 0.7	2.0 ± 0.4	0.4 ± 0.1	0.8 ± 0.1	1.5 ± 0.5	1.2 ± 1.2	
CO ₂ :								
$\sigma_{q, q-1}$	1.1 ± 0.1	5.1 ± 1.0	7.1 ± 0.6	4.1 ± 0.5	6.8 ± 1.4	6.3 ± 0.7	7.2 ± 1.8	
$\sigma_{q,q-2}$	1.2 ± 0.1	1.3 ± 0.6	2.6 ± 0.4	0.6 ± 0.1	1.1 ± 0.2	2.1 ± 0.5	2.0 ± 1.7	
Häberli et al. $\sigma_{a, a-1}$								
Wegmann et al. $\sigma_{q, q-1}$		5	12	2	12			

^a Cross sections are in units of 10⁻¹⁵ cm².

different proposed mechanisms. Even if charge exchange is not the dominant process, spectral lines from these reactions will still be observed and associated with individual solar wind ions. Other mechanisms result in broadband X-ray emission.

Since the gasdynamics of the comet's coma can be well determined from longer wavelength observations, reliable data on the charge exchange could allow comets to be used to monitor accurately the composition of the solar wind, as has been suggested by Dennerl et al. (1997). To this end, we have developed an experiment to measure total charge-exchange cross sections for collisions of highly charged states of C, N, O, and Ne with the comet-abundant species H₂O and CO₂. We previously reported measurements of cross sections for hydrogen and helium ion interactions with H₂O and CO₂ (Greenwood, Smith, & Chutjian 2000). These results were of interest to observations of solar wind ion depletion as a function of distance from comet Halley by the Ion Mass Spectrometer/High-Energy Range Spectrometer instrument on the Giotto spacecraft (Shelley et al. 1987; Fuselier et al. 1991). In the present work, we have installed a detector to observe X-ray emissions from the charge-exchange collisions, leading to the more sensitive measurement of line-emission cross sections.

2. EXPERIMENTAL DETAILS

The apparatus and method used to measure total charge-exchange cross sections has been described previously (Greenwood et al. 2000), but a brief description will be given here. To produce beams of highly charged ions present in the solar wind, an electron cyclotron resonance ion source (Liao et al. 1997; Chutjian, Greenwood, & Smith 1999) is employed. Individual species are accelerated and mass/charge selected using a double-focusing 90° analyzing magnet. The ions then pass through a target cell filled with gas (H₂O or CO₂) at a pressure low enough to ensure single-collision conditions. The final charge state of the ion after a reaction is determined by a retarding potential technique. By measuring the pressure in the collision cell using a capacitance manometer, absolute cross

TABLE 2
LABORATORY ION
COLLISION VELOCITIES

Ion	Velocity (km s ⁻¹)			
¹³ C ³⁺	558			
¹³ C ⁶⁺	789			
$^{15}N^{7+}$	794			
¹⁶ O ⁵⁺	650			
¹⁸ O ⁷⁺	724			
¹⁸ O ⁸⁺	774			
²² Ne ⁹⁺	743			
²² Ne ¹⁰⁺	783			

sections for the process are obtained. Recently, a high-purity germanium X-ray detector has been installed to observe photons emitted at angles close to 90° to the ion beam direction. A 7.5 μ m—thick beryllium window protects the detector from contamination while allowing transmission of energetic photons. The window transmission is less than 0.5% at 400 eV, rising to 4% at 600 eV, 20% at 800 eV, and 40% at 1000 eV. The minimum detector resolution of about 100 eV is narrow enough to allow separation of the $2p \rightarrow 1s$, $3p \rightarrow 1s$, and $4p \rightarrow 1s$ transitions in the ions studied.

3. RESULTS

Total cross sections for single (j = 1 in eq. [1]) and double (j = 2) charge exchange of C^{3+} , C^{6+} , N^{7+} , O^{5+} , O^{7+} , O^{8+} , and Ne^{9+} in H_2O and CO_2 are presented in Table 1. Also included are cross sections used by Häberli et al. (1997) and Wegmann et al. (1998) in their models. All measurements were made at collision energies of 7q keV, where q is the ionic charge. The corresponding velocities are shown in Table 2.

X-ray spectra obtained from collisions of Ne^{10+} , Ne^{9+} , O^{8+} , O^{7+} , and N^{7+} with H_2O and CO_2 were acquired. Spectra of Ne^{10+} , Ne^{9+} , and O^{8+} in H_2O are shown in Figure 1 and are uncorrected for transmission of the Be window. For Ne^{10+} and Ne^{9+} , the main peak (resulting from $2p \rightarrow 1s$ transitions) is well enough separated from other contributions to determine a FWHM of 104 eV. Gaussian peaks centered on the known transition energies were fitted to the data, and relative contributions were determined. The transmission efficiency of the Be window was applied to the deconvoluted peaks. Results are presented in Tables 3 and 4.

For each collision, only one photon is emitted in the energy range of the detector. The relative contributions in the X-ray spectra can be normalized by using the measured single charge-exchange cross sections. The line-emission cross sections obtained are shown in Table 3. It is known from other work that capture occurs mainly into the n=4, 5 states. Hence, all of the $2p \rightarrow 1s$ transition arises via cascade from higher levels. Also, a small correction (15%) was made to account for collisions that populate the 2s metastable state of the ion, since this will decay outside the viewing length of the detector. This value was determined by analysis of cascading pathways of an ion that has captured an electron into an n=4 or 5 state (Wiese, Smith, & Miles 1969). Full details of the above procedures will appear in a forthcoming publication.

X-ray emission from double charge exchange also occurs. The low-energy shoulder on the main peak of the Ne¹⁰⁺ spectrum is probably from Ne⁸⁺ emission following capture of two electrons. Although the ions we studied generate X-rays at energies higher than the peak observed in most comets to date (200–300 eV), Owens et al. (1999) and Dennerl et al. (1997)

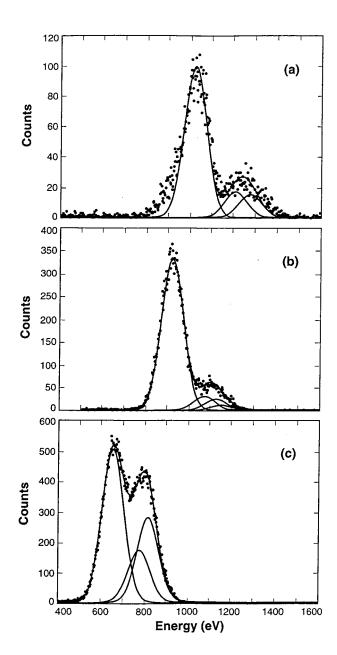


FIG. 1.—X-ray spectra (uncorrected for the transmission of the Be window) obtained from collisions of (a) $^{22}\text{Ne}^{10+}$, (b) $^{22}\text{Ne}^{9+}$, and (c) $^{18}\text{O}^{8+}$ with H₂O. The transitions, from lower to higher energy, correspond to the $np \rightarrow 1s$ series for n=2,3, and 4 (and for n=2,3,4, and 5 for Ne $^{9+}$).

have shown that there is significant emission at energies ≥ 1 keV. During periods of increased solar activity, the solar wind might be expected to contain more highly charged species.

4. DISCUSSION

The results in Table 1, which compare our experimentally measured cross sections and those used by Häberli et al. and Wegmann et al., show up to a factor of 2 difference. This highlights the problem with using semiclassical models or trying to deduce cross sections that have not been previously measured or accurately calculated. It is also noted that double charge-exchange cross sections cannot be ignored in models. They can be as much as 35% of single exchange for highly charged ions. For the case of C³⁺, the double and single cross sections are found to be equal.

An important consideration arising from the X-ray spectra is that the $2p \rightarrow 1s$ transition is found to dominate the spectra (comprising 70%–90% of the total spectrum). The assumptions of Häberli et al. on line intensity ratios result in 100% contribution from $2p \rightarrow 1s$, while for Wegmann et al. it is 25% following capture into n = 4. The effectivity f has also been used to estimate the fraction of collisions that produce an X-ray photon. In a single charge-exchange reaction, one captured electron radiatively stabilizes and emits one X-ray photon for the ions studied. Therefore, a value f = 1 should be used in conjunction with the measured cross sections. If the density of gas in the coma is sufficiently high and the lifetime of the 2s metastable state is long, then it is possible that the 2s state will be populated and subsequently collisionally quenched, thus reducing f. However, f will still be greater than 0.85. The present measurements should prove valuable in helping to resolve some of these issues.

5. CONCLUSIONS

Total single and double charge exchange and X-ray lineemission cross sections have been measured for high charge states of C, N, O, and Ne ions interacting with H₂O and CO₂ at velocities between 550 and 800 km s⁻¹. The double chargeexchange cross sections were found in several cases to be comparable to those for single exchange, and in C³⁺ the double and single cross sections were found to be equal. X-ray emission cross sections were obtained from the measured chargeexchange data, with correction for collisions which populate the metastable 2s levels. Present measurements will enable future efforts to be more detailed in their treatments, particularly in the determination of X-ray line intensities from comets. With the current and projected launch of X-ray satellites, comparisons with higher resolution observations should soon be possible. We intend to investigate X-ray line emission in charge

TABLE 3

Line-emission Cross Sections and Relative Contributions for X-Ray Emission From Collisions of Solar Wind Ions with H.O.

	N^{7+}			O^{7+}			O_{8+}			Ne ⁹⁺			Ne ¹⁰⁺	
Transition	Energy Level (eV)	Cross Section ^a	Relative Contrib. (%)	Energy Level (eV)	Cross Section ^a	Relative Contrib. (%)	Energy Level (eV)	Cross Section ^a	Relative Contrib. (%)	Energy Level (eV)	Cross Section ^a	Relative Contrib. (%)	Energy Level (eV)	Relative Contrib. (%)
$\sigma(2p-1s)$	500	3.4 ± 1.8	42	574	3.2 ± 0.5	70	654	4.2 ± 0.5	77	922	6.2 ± 1.5	91	1022	81
$\sigma(3p-1s)$		2.6 ± 1.4	32	666	0.6 ± 0.2	13	775	0.5 ± 0.2	10	1074	0.27 ± 0.12	4	1211	10
$\sigma(4p-1s) \ldots \sigma(5p-1s) \ldots$	625 640	2.1 ± 1.2 ^b	26 ^b	698 713	$0.8 \pm 0.2^{\text{b}}$	17 ^b	817 837	$0.7 \pm 0.2^{\text{b}}$	13 ^b	1127 1152	0.20 ± 0.10 0.14 ± 0.07	2	1277 1308	9 ^b

Note. - Energy levels are from Kelly 1982. The relative contribution of each transition is given as deconvoluted from spectra such as shown in Fig. 1.

^a Units of cross section are 10⁻¹⁵ cm².

^b Cross sections and relative contributions are for the combined $\sigma(4p-1s)$ and $\sigma(5p-1s)$ transitions.

TABLE 4 LINE-EMISSION CROSS SECTIONS AND RELATIVE CONTRIBUTIONS FOR X-RAY EMISSION FROM COLLISIONS OF SOLAR WIND IONS WITH CO.

	O^{7+}			O_{8+}				Ne ⁹⁺	Ne ¹⁰⁺		
Transition	Energy Level (eV)	Cross Section ^a	Relative Contribution (%)	Energy Level (eV)	Cross Section ^a	Relative Contribution (%)	Energy Level (eV)	Cross Section ^a	Relative Contribution (%)	Energy Level (eV)	Relative Contribution (%)
$\sigma(2p-1s)$	574	4.2 ± 0.9	73	654	4.1 ± 0.5	76	922	5.6 ± 1.4	92	1022	81
$\sigma(3p-1s)$	666	0.8 ± 0.3	13	775	0.5 ± 0.2	10	1074	0.24 ± 0.11	4	1211	11
$\sigma(4p-1s)$	698	b	b	817	b	b	1127	0.12 ± 0.06	2	1277	b
$\sigma(5p-1s)$	713	0.8 ± 0.3^{b}	14 ^b	837	0.8 ± 0.2^{b}	14	1152	0.12 ± 0.06	2	1308	8 ^b

NOTE. - Energy levels are from Kelly 1982. The relative contributions of each transition are given as deconvoluted from spectra such as shown in Fig. 1.

exchange for different velocities and to extend both the range of projectile ions and charge states studied, as well as the cometary neutral targets.

We thank R. Häberli for cross sections used in his comet Xray modeling. This work was carried out at the Jet Propulsion Laboratory/Caltech and was funded by the JPL Director's Discretionary Fund and NASA. J. B. G. acknowledges the support of the National Research Council through the Associateships Program and the Queen's University Belfast Research Fund. I. D. W. acknowledges support of both EPSRC and the QUB Research Fund.

REFERENCES

Bame, S. J. 1972, in Solar Wind, ed. C. P. Sonett, P. J. Coleman, Jr., & J. M. Wilcox (NASA SP-308; Washington, DC: NASA), 535

Boschler, P. 1987, Phys. Scr., T18, 55

Chutjian, A., Greenwood, J. B., & Smith, S. J. 1999, in Applications of Accelerators in Industry, ed. J. L. Duggan & I. L. Morgan (New York: AIP),

Cravens, T. E. 1997, Geophys. Res. Lett., 24, 105

Dennerl, K., Englhauser, J., & Trumper, J. 1997, Science, 277, 1625

Dijkkamp, D., Gordeev, Y. S., Barzuk, A., Drentje, A. G., & de Heer, F. J. 1985, J. Phys. B, 18, 737

Fuselier, S. A., Shelley, E. G., Goldstein, B. E., Goldstein, R., Neugebauer, M., Ip, W.-H., Balsiger, H., & Reme, H. 1991, ApJ, 379, 734

Greenwood, J. B., Smith, S. J., & Chutjian, A. 2000, ApJ, 529, 605

Häberli, R. M., Gombosi, T. I., De Zeeuw, D. L., Combi, M. R., & Powell, K. G. 1997, Science, 276, 939

Kelly, R. L. 1982, Atomic and Ionic Spectral Lines (Oak Ridge National Lab. Report ORNL-5922)

Krasnopolsky, V. 1997, Icarus, 128, 368

Liao, C., Smith, S. J., Chutjian, A., & Hitz, D. 1997, Phys. Scr., T73, 382 Lisse, C. M., et al. 1996, Science, 274, 205

Mann, R., Folkmann, F., & Beyer, H. F. 1981, J. Phys. B, 14, 1161

Owens, A., et al. 1999, Nucl. Phys. B, 69, 735

Phaneuf, R. A., Alvarez, I., Meyer, F. W., & Crandall, D. H. 1982, Phys. Rev. A, 26, 1892

Shelley, E. G., et al. 1987, A&A, 187, 304

Wegmann, R., Schmidt, H. U., Lisse C. M., Dennerl, K., & Englhauser, J. 1998, Planet. Space Sci., 46, 603

Wiese, W. L., Smith, M. W., & Miles, B. M. 1969, Atomic Transition Probabilities, National Standard Reference Data Series, Vol. II (National Bureau of Standards Circ. 22; Washington, DC: Gov. Printing Office)

^a Units of cross section are 10⁻¹⁵ cm².

^b Cross sections and relative contributions are for the combined $\sigma(4p-1s)$ and $\sigma(5p-1s)$ transitions.